Carbazole-2-carbonitrile, 5,6,7,8-tetrahydro-1-methyl-

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 165 °C

Global applicability domain: Inside

Local applicability domain index: 4.81e-01

Confidence level: 3.73e-01

Nearest Neighbors from the Training Set

Image not found
Bendazol [INN:DCF]
Measured: 187
Predicted: 187

Image not found
2-Phenylbenzimidazole
Measured: 293
Predicted: 195

Image not found
4-cyanoquinoline
Measured: 104
Predicted: 89.8

Image not found
Quinoline-3-carbonitrile
Measured: 109
Predicted: 89.8